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Hidden Fermi surface in $K_xFe_{2-y}Se_2$: LDA + DMFT study

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Investigation of the superconductivity in recently discovered iron-based superconductors is one of the main trends in modern condensed matter physics. Some of iron chalcogenide superconductors [1] have qualitatively different electronic properties from other iron-based superconductors (e.g., iron pnictides). Among them, the $K_xFe_{2-y}Se_2$ compound and the FeSe monolayer on the $SrTiO_3$ substrate take quite a special place. Early days angular resolved photoemission spectra (ARPES) experiments showed that for these compounds there are absent or practically can not be resolved hole-like Fermi surface sheets near the Γ-point of the Brillouin zone. While for the iron pnictides and some iron chalcogenides (e.g. bulk FeSe) these hole-like Fermi surface sheets near the Γ-point were clearly observed by ARPES. The absence of the hole-like Fermi surface sheets near the Γ-point indicates that for $K_xFe_{2-y}Se_2$ series there is no possibility of nesting between the hole sheets of the Fermi surface near the Γ-point and electronic sheets near the X-point. Thus a spin-fluctuation mechanism of superconducting pairing (assumed for iron pnictides [2]) is not applicable here.

Recently in the work [3] ARPES observation of a hidden hole-like band approaching the Fermi level near the Γ-point for the $K_{0.62}Fe_{1.7}Se_2$ system was reported. Also in the work [3] on the basis of the ARPES data analysis there was proposed a presence of a hidden hole-like Fermi surface near the Γ-point. The authors of [3] provide some reasons why the Fermi surfaces near the Γ-point previously were not observed due to the geometry of the experiment.

The computational methodological LDA + DMFT details could be found in our earlier works [4, 5] on $K_xFe_{2-y}Se_2$ material. Further we provide specific details of the LDA+DMFT calculations. The DMFT(CT-QMC) computations were done at reciprocal temperature $\beta = 40$ (~ 290 K) with about 10^8 Monte-Carlo sweeps. Interaction parameters of Hubbard model were taken $U = 3.75$ eV, $J = 0.56$ eV [8]. We employed the self-consistent fully-localized limit definition of the double-counting correction [7]. Thus computed values of Fe-3d occupancies and corresponding double-counting energies are $E_{dc} = 18.50$, $n_d = 5.66$ ($K_{0.62}Fe_{1.7}Se_2$).

The LDA + DMFT spectral function maps were obtained after analytic continuation of the local self-energy $\Sigma(\omega)$ from Matsubara frequencies to the real ones. To this end we have applied Pade approximant algorithm [9] and checked the results with the maximum entropy method [10] for Green's function $G(\tau)$.

In the Figure 1 we present comparison of ARPES Fermi surface maps from [3] (panels (a), (c), (e)) with our theoretical LDA′ + DMFT data (panels (b), (d), (f)). Experimental data [3] (panels (a), (c), (e)) is given for three different offset energies with respect to experimental Fermi level energy – 0, −20, and −40 meV. On the panel (a) experimentalists see one Fermi surface sheet near X-point. For the Fermi surface sheet around X-point there are many experimental points shown by blue dots which finally form a circle like sheet (drawn by blue line to guide eyes). The same situation is also seen on panels (c) and (e) with narrowing of the sheet upon going away from the Fermi level. This picture coincides with many other experimental papers (see, e.g., review [1]). A similar behavior near X-point can be noted for LDA + DMFT results on panels (b), (d) and (f). However LDA+DMFT gives two small Fermi sheets here, which probably are not resolved by ARPES.

The situation in the vicinity of the Γ-point is physically much more interesting. The authors of the [3] claim that there are two Fermi surface sheets near Γ-point marked as α and β (see Fig. 1a). Those α and β sheets the authors of the [3] call as a hidden Fermi surface. However for the Fermi surface sheet around Γ-point there are only four points for which expermintalists assume a circular shape of the sheet (drawn by blue line to guide eyes) as a simplest possible choice. But if we look at panel (b) containing LDA + DMFT data it immediately appears that around Γ-point there are four quite small "propeller" like Fermi surface sheets. Surprisingly, if we map experimental blue dots from panel (a) to theoretical Fermi surface map (panel (b)) those dots perfectly coincides with "propellers". Thus one can conclude that indeed around Γ-point there is a manifestation of the Fermi surface with more complicated

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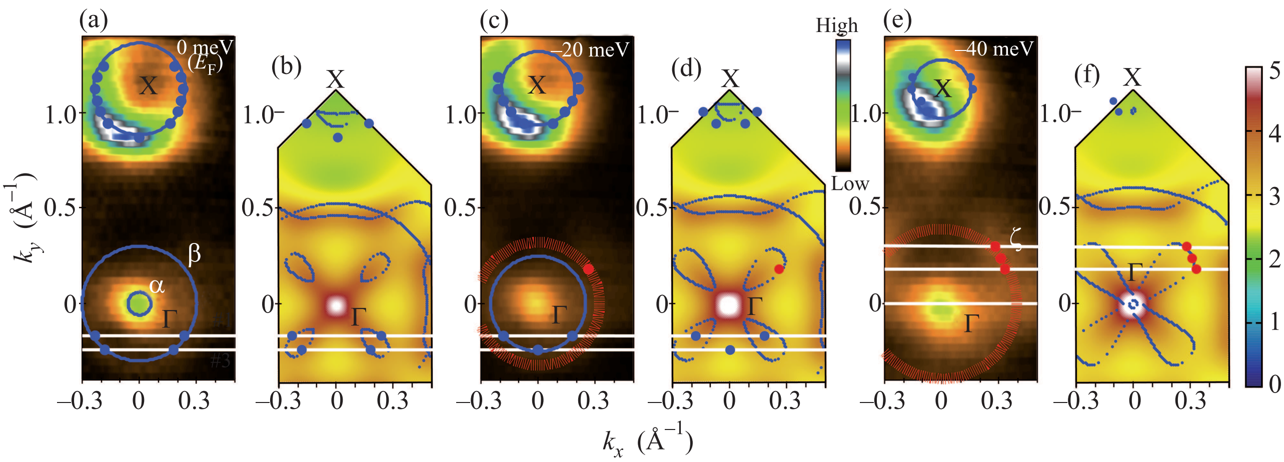

Fig. 1. (Color online) (a), (c), (e) – ARPES Fermi surface maps for $K_{0.62}Fe_{1.7}Se_2$ [3] plotted with different offset energies with respect to experimental Fermi level energy with Fermi surface sheets shown by dots and lines to guide eyes. (b), (d), (f) – LDA′ + DMFT Fermi surface maps with maxima of corresponding spectral function shown by small blue dots. Big blue and red dots on (b), (d), (f) panels correspond to dots on (a), (c), (e) panels

shape in contrast to a circular one suggested in [3]. If we now turn to the tiny α sheet on panel (a) of Fig. 1 one can observe rather a halo like structure than a circle one. On the panel (b) one can find identical halo at the Γ-point which is formed because of summation of intensities coming from the "propeller" blades. So the work of [3] shows perhaps for the first time a presence of a hidden hole like Fermi surface near Γ-point for KFeSe-class of systems. Similar behavior can be observed of the panels (c), (d) and (e), (f).

To conclude, here on the basis of the works [4, 5] and inspired by the work of [3] we confirm within our LDA + DMFT calculations that for $K_{0.62}Fe_{1.7}Se_2$ system near the Γ-point there are the hidden Fermi surface sheets. Also it is demonstrated that correlation effects are more important for KFeSe-supercoductors than for FeAs-based materials in a sense of Fermi surface formation. Its appearance can justify spin-fluctuation mechanism of superconductivity in this class of systems with a rather high critical temperature $T_c \sim$30K. Good qualitative and even quantitative agreement of the calculated and ARPES Fermi surfaces is obtained.

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